WRF-Chem (V3.4): A summary of status and updates

Georg Grell

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\+ *many more national and international collaborators*

WRF/Chem web site - http://wrf-model.org/WG11

Structure of talk

- What is new in WRF/Chem – V3.4
- Ongoing and future work

Adding Gas Phase Chemistry and Aerosol Packages (all implemented by **ESRL**)

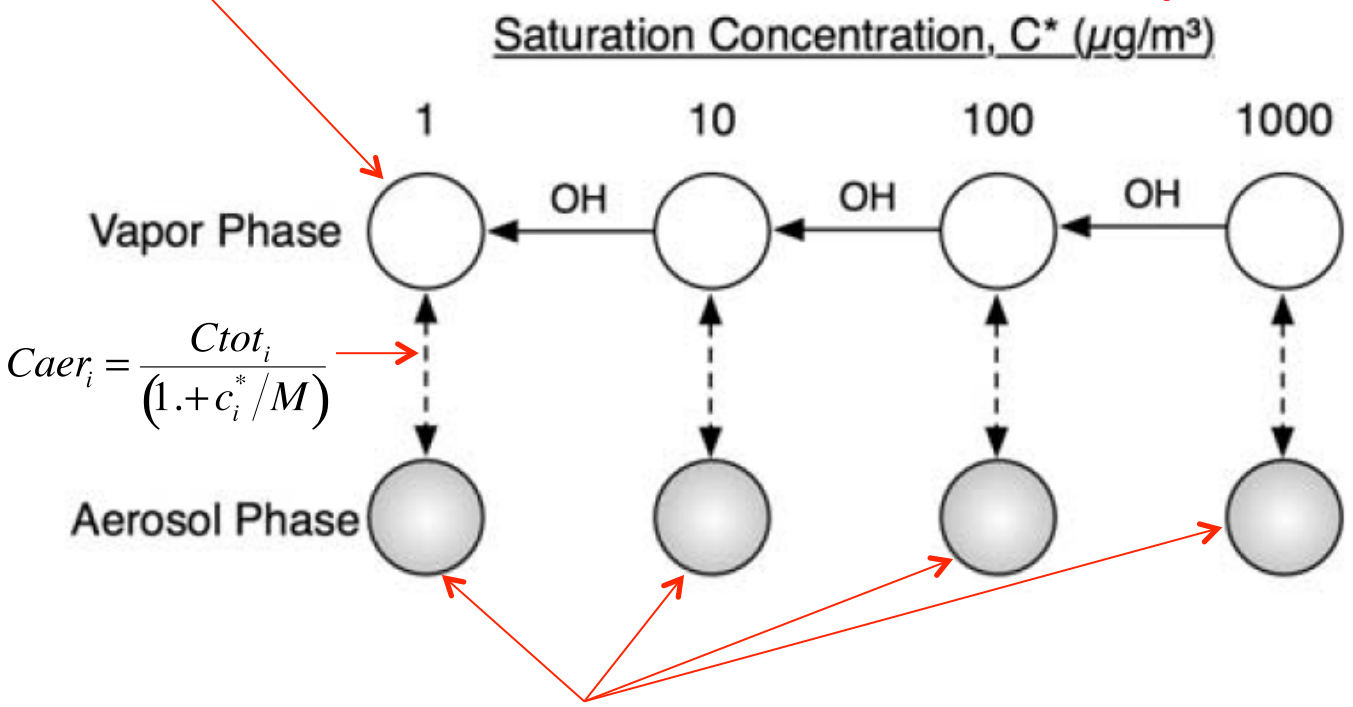
- New gasphase chemistry packages using the Kinetic Pre Processor (KPP) include
  - RACM and/or RADM with MADE/SORGAM coupled with aerosol indirect effect and simple aqueous phase chemistry (CMAQ AQCHEM routine)
  - RACM – MADE/VBS-SOA (SORGAM was replaced by Volatility Basis Set (VBS) approach)

Volatility Basis Set (VBS) Approach for MADE (modal scheme)

8 Organic Aerosol Species: Optimized for OA bias removal and run-time efficiency

Organic condensable vapors (OCVs)

from Farina et al., 2010



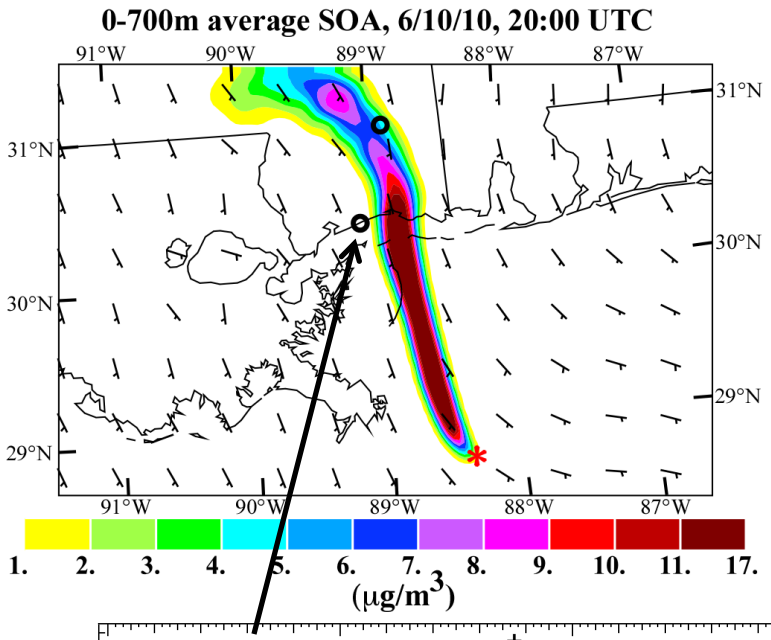
Secondary Organic Aerosol (SOA)

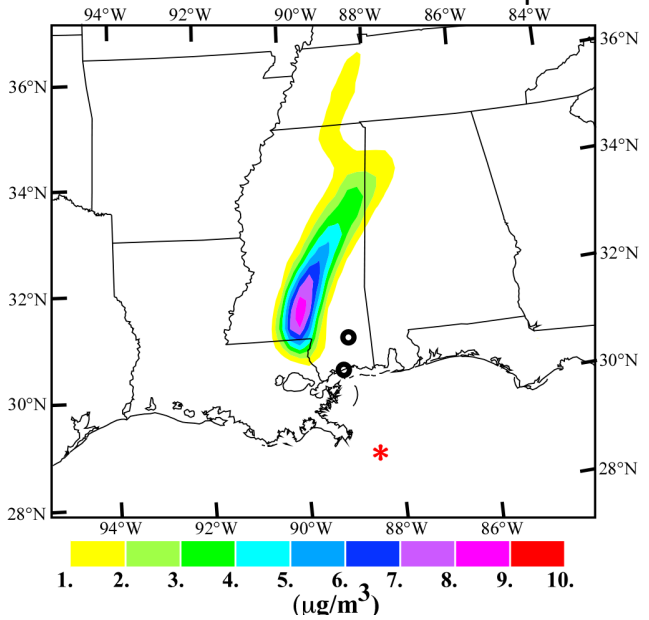
"Aging" takes place in the gas phase OCV reactions with OH, deposition of these vapors can be significant removal mechanism.

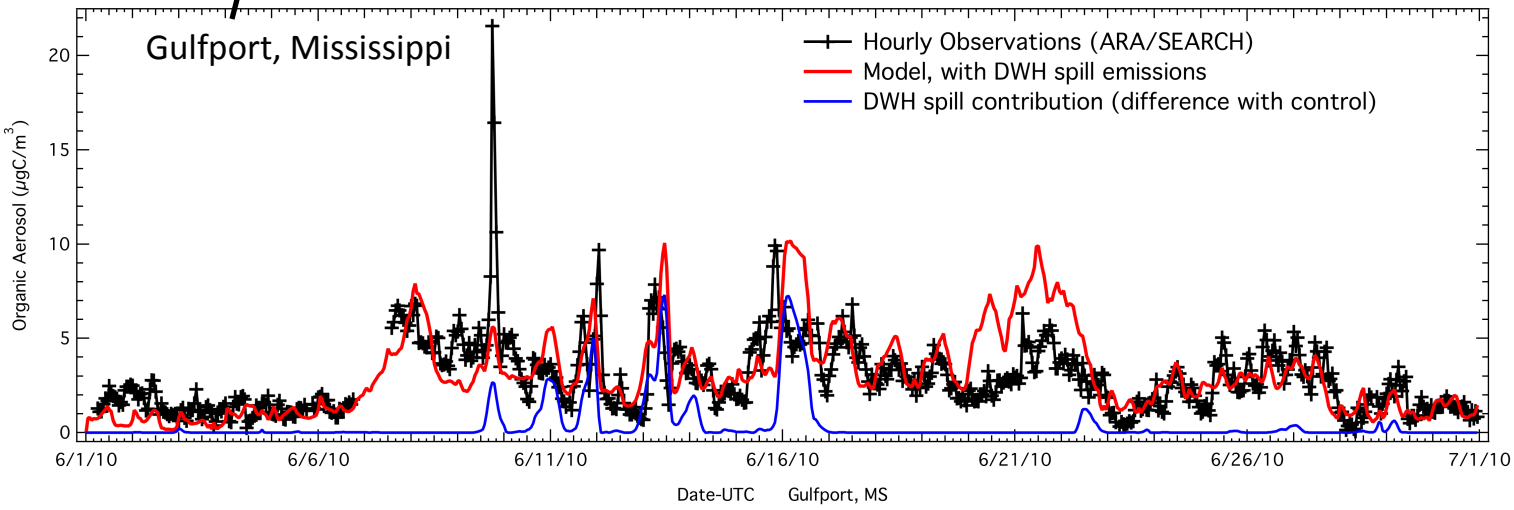
The Volatility Basis Set Approach to SOA
Application to the Deepwater Horizon Oil Spill

(Middlebrook et al., 2011, PNAS)

6/12/10, 10:00 UTC, maximum DWH impact North of 31°
Surface SOA from DWH oil spill







WRF-Chem Greenhouse Gas Packages *(chem_opt =17)-new in WRF-ChemV3.4*

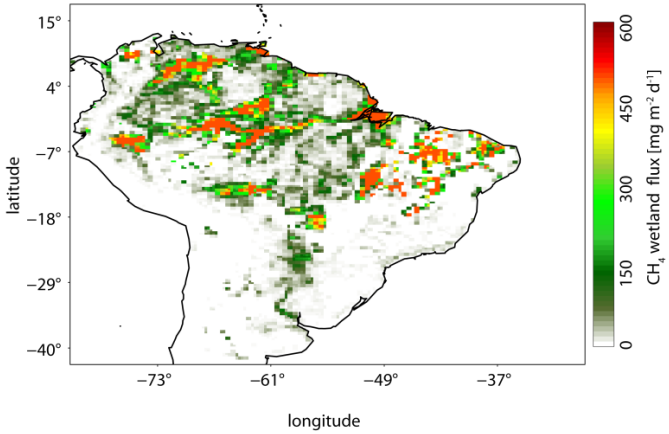
- **Online calculation of biospheric CH_4 fluxes**
  wetland – Kaplan (2002)
  termite – Sanderson (1996)
  soil uptake – Ridgwell et al. (1999)

- **Passive tracer simulations for CO_2, CH_4, and CO**
  (including all options of CO_2 tracer package, chem_opt=16)

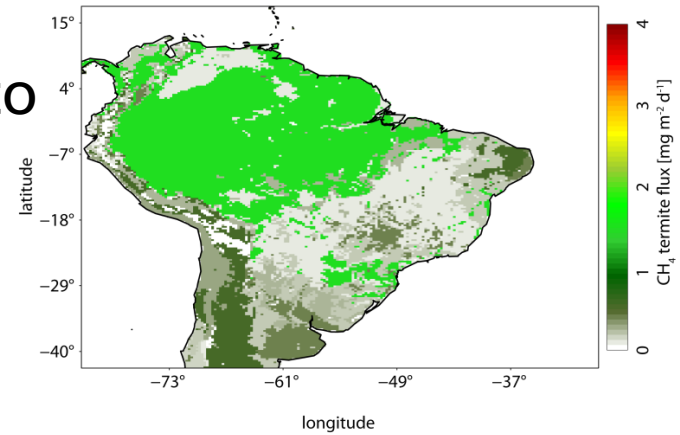
- **Tuning of wetland fluxes** through namelist options wpeat and wflood possible

- **Separate biomass burning option** for CO_2, CH_4, and CO including plumerise calculation (biomass_burn_opt = 5)

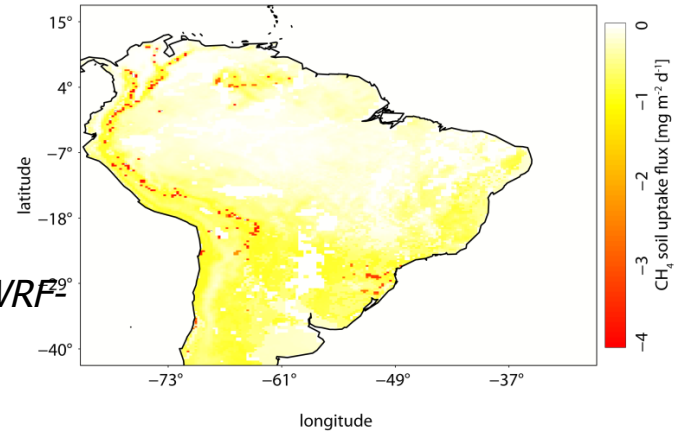
- **Detailed description**
  Beck et al., (2011): The WRF Greenhouse Gas Model (WRF-GHG) Technical Report No. 25, Max Planck Institute for Biogeochemistry, Jena, Germany, available online at http://www.bgc-jena.mpg.de/bgc-systems/index.shtml



wetland CH_4 flux



termite CH_4 flux



soil uptake CH_4 flux

A new dust model (dust_opt=3)

AFWA/AER Dust scheme – modeled after GOCART approach, but included is sand blasting component and clay dependence

- Bulk Vertical Dust Flux Scheme: Based on Marticorena & Bergametti (1995)
  - Threshold Friction Velocity (Iversen & White, 1982)):

$$u_{*_t}(D_p) = 0.129 \frac{\left[\frac{\rho_p g D_p}{\rho_a}\right]^{0.5}\left[1+\frac{0.006}{\rho_p g D_p^{2.5}}\right]^{0.5}}{\left[1.928\left(aD_p^x+b\right)^{0.092}-1\right]^{0.5}} \qquad u_{*_t} = u_{*_t}(D_p)\frac{f(\text{moisture})}{f(\text{roughness})}$$

  - Saltation Flux Over Bare Soil (Kawamura, 1951):

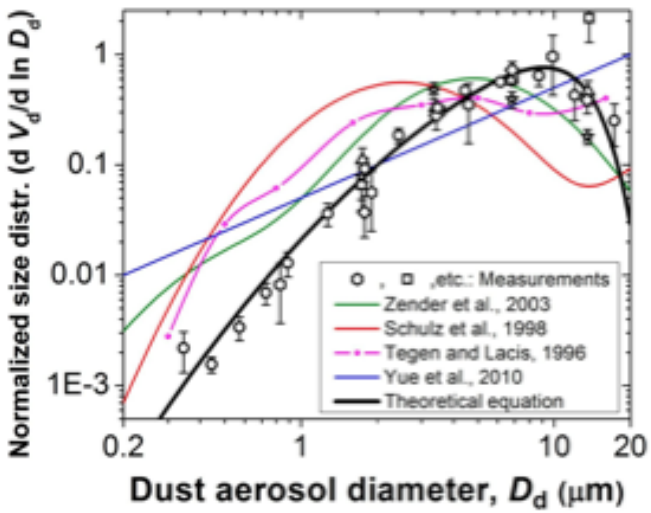
$$H(D_p) = C\frac{\rho_a}{g}u_*^{\,3}\left(1+\frac{u_{*_t}}{u_*}\right)\left(1-\frac{u_{*_t}^{\,2}}{u_*^{\,2}}\right) \qquad G = \sum H(D_p)\,dS_{rel}(D_p)$$

  - Bulk Vertical Dust Flux (efficiency factor (α): Gillette, 1979)

$$F_{bulk} = G\alpha \times \text{Erod} \qquad \alpha = 10^{0.134(\%\text{clay})-6}$$

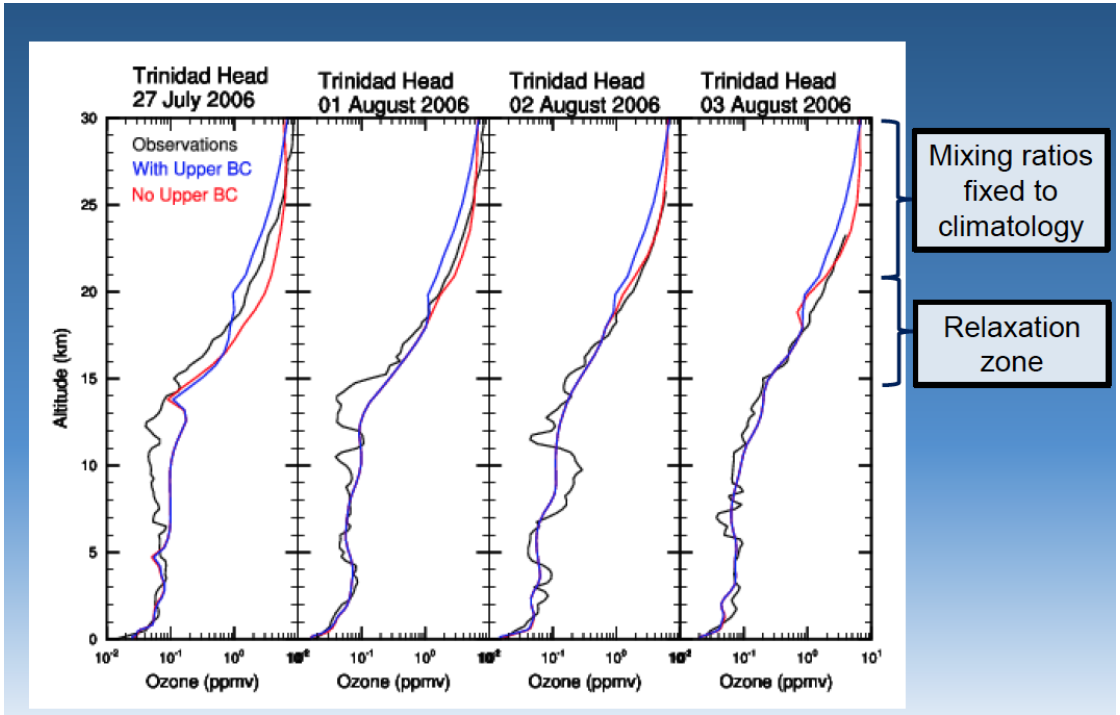
AFWA/AER Dust scheme

- Particle Size Distribution developed by Jasper Kok (NCAR)
  - Brittle material fragmentation theory
  - Kok, 2010
- *f*(roughness) is a drag partition correction
- *f(moisture)* calculated using Fecan's (Fecan et al. 1999) method, incorporates soil texture, increases u^*_t as soil moisture increases



NCAR/ACD Updates to WRF-V3.4

- Wet Deposition for MOZART gas species following Neu et al. (2011)
- Upper Chemical Boundary Conditions (Past/Present/Future UBC from WACCM climatology)
- MOZART/MOSAIC w. simplified SOA scheme
- Output tracking tool
- Lightning NO production for parameterized convection
- Various bug fixes (including a versatile bioemdt setting for MEGAN)



NCAR/ACD Updates to Preprocessing Tools

http://web3.acd.ucar.edu/wrf-chem/

- All preprocessing tools now work on Lambert, Polar, Mercator and Lat/Lon projections
- mozbc updated to include time interpolation

For questions on updates from NCAR/ACD contact Mary Barth, Gabriele Pfister, Alma Hodzic, Stacy Walters, John Wong

Fires and Volcanoes: What's new in V3.4

Volcanic ash in WRF-Chem V3.4

- Additional options for transport only (4 bins), transport + ash-fall (10 bins +so2 + so4)
- Coupled with some chemistry/aerosol modules (only using up to three bins – depending on size), interaction with meteorology included for these options
- Evaluation with aircraft, satellite, and lidar data from Eyjafjallajökull 2010

10 size bins for prediction of ash-fall and transport of volcanic ash

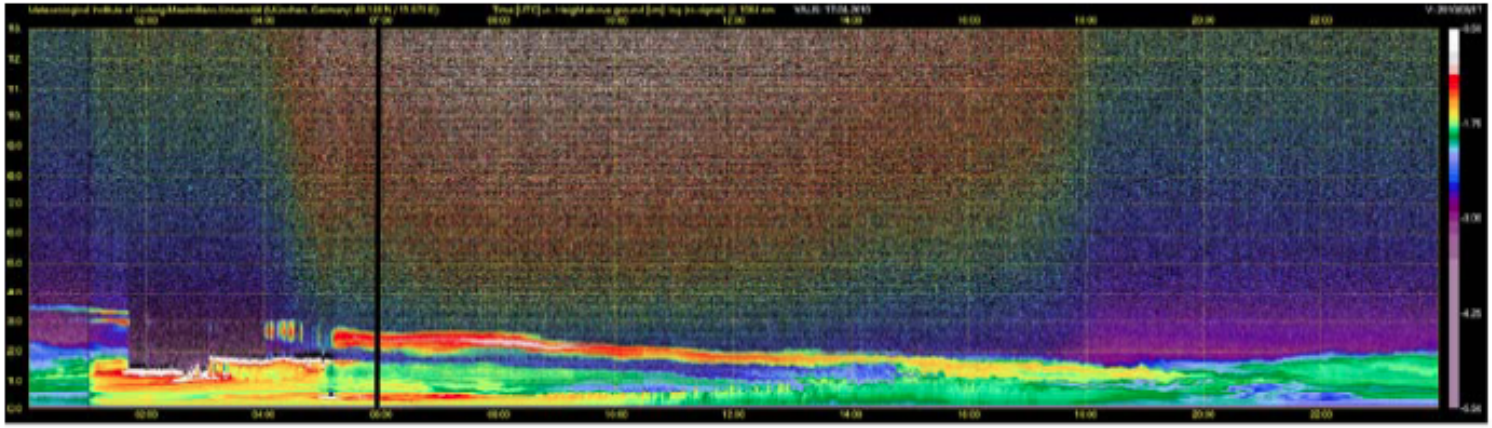
Particle Size Bin	Phi	Percentage of mass
1 – 2mm	-1 – 0	2
0.5 – 1 mm	0 – 1	4
0.25 – 0.5 mm	1 – 2	11
125 – 250 µm	2 – 3	9
62.5 – 125 µm	3 – 4	9
31.25 – 62.5 µm	4 – 5	13
15.625 – 31.25 µm	5 – 6	16
7.8125 – 15.625 µm	6 – 7	16
3.9065 – 7.8125 µm	7 – 8	10
< 3.9 µm	> 8	10

4 size bins for prediction if transport only is of interest

Particle Size Bin	Phi	Percentage of mass
15.625 – 31.25 µm	5 – 6	16
7.8125 – 15.625 µm	6 – 7	16
3.9065 – 7.8125 µm	7 – 8	10
< 3.9 µm	> 8	10

3 size bins for coupling with other aerosol modules

Forecast compared to Munich Lidar, April 17, 06Z



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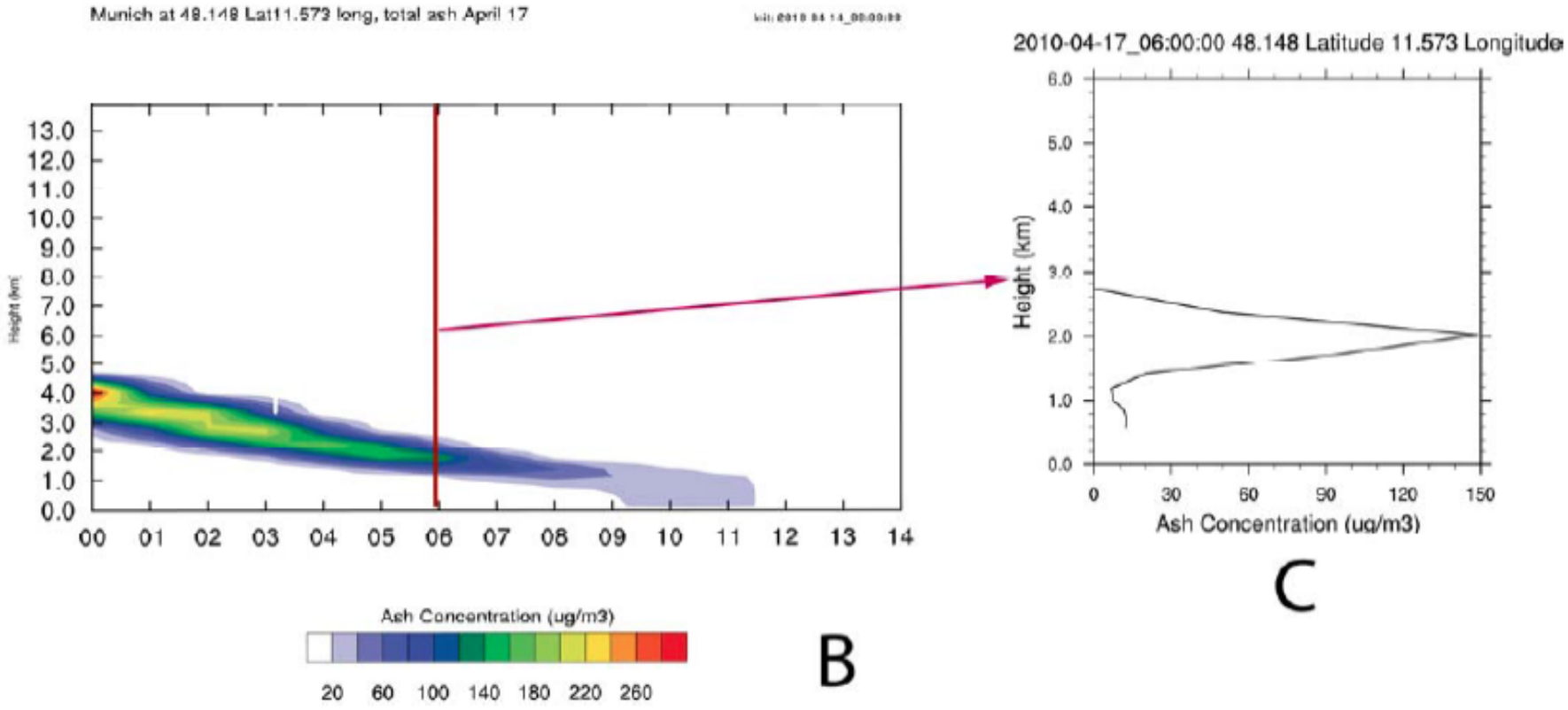


Other additions

- CMAQ AQCHEM routine was fixed and is now used for aqueous phase chemistry in the convective parameterization (namelist option conv_tr_aqchem, defaults to “1”)
- CMAQ-AQCHEM can also be used for explicit microphysics (chem_opt 40 and 41)
- Wet scavenging for aerosols, so2, so4, sulf, nh3, and hno3 in convective parameterization is now made optional (conv_tr_wetscav, defaults to “1”)

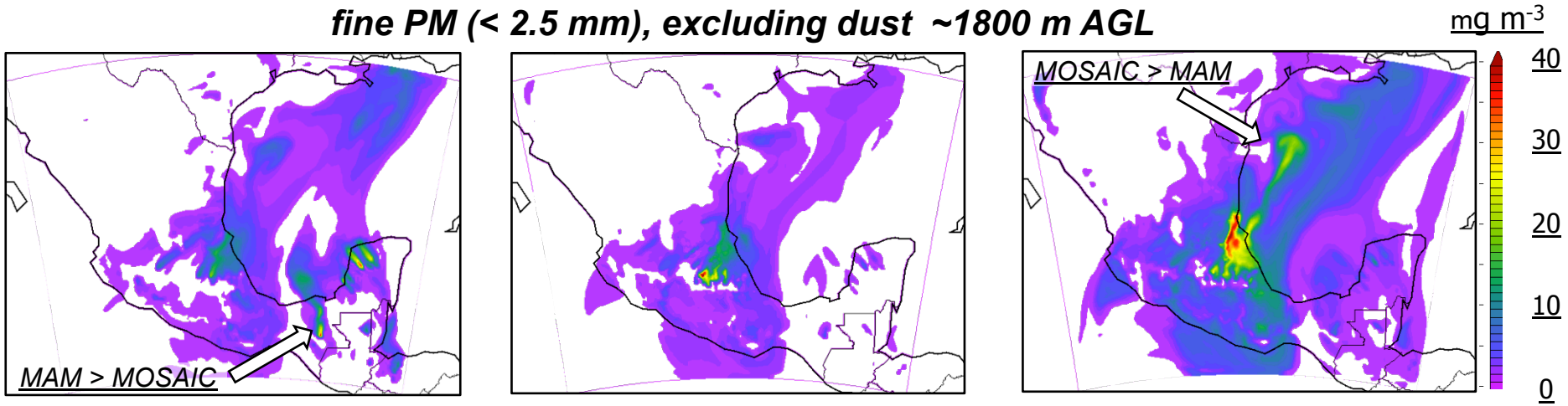
PNNL future addition: Aerosol Model from CAM5 Ported to WRF-Chem

MAM (from CAM5)
modal – 3 modes, **18** species
'simple'
1 simulation day ~ 21 min

MADE/SORGAM
modal – 3 modes, **38** species
9 times more species
~ 24 min

MOSAIC
sectional – 4 bins, **164** species
'complex'
~ 60 min

fine PM (< 2.5 mm), excluding dust ~1800 m AGL



- Identical emissions, meteorology, chemistry, dry deposition, boundary conditions
- Differences due to secondary aerosols (SO_4, NO_3, NH_4, organics)
- Treatment of organics:
- **MAM**: POA - non-volatile, SOA – simple yields
- **MADE/SORGAM**: POA - non-volatile, SOA - 2-product approach
- **MOSAIC**: 'volatility basis set' approach, volatile POA & SOA

WRF/Chem ongoing and future work – PNNL

1. Morrison-Gettleman microphysics coupled to aerosols
2. Aerosol resuspension treatment
3. Alternative treatments for cloud-aerosol interactions
4. Treatment of aerosol-cloud interactions and cloud chemistry in shallow and deep convective parameterizations (for larger scale simulations)
5. New particle formation treatment
6. Simplified photochemical mechanism (half the speed of CBM-Z) coupled with MAM and MOSAIC.

(1) Will probably make it into V3.5, (2) – (6) are questionable

WRF/Chem ongoing and future work – PNNL

- Aerosol modeling test bed is still in the works and making progress

http://www.pnl.gov/atmospheric/research/aci/amt/index.stm

- Some of the Analysis Toolkit Software available via the web site
- MILAGRO test bed data is finished,
- CHAPS, VOCALS, ISDAC/ARCTAS, CARES/CalNex integrated datasets (field campaign + routine monitoring) planned for the future

WRF/Chem current and future work – ESRL + other groups

- Aerosols were coupled with convective parameterization (G3, collaboratively with S. Freitas)
- Volcanic emissions will be added to more aerosol modules
- Using WPS to run WRF-Chem off global FIM-Chem
- 2008 EPA emissions (US)
- Improved global emissions (prep_chem_sources)
- Aerosol-microphysics interactions for RACM_MADE_SOA_VBS
- Including isoropia2 (MADE related aerosol modules)
- NASA: coupling GOCART with microphysics, also with new GODDARD radiation scheme

NCAR/ACD Future Updates

- WRF-Chem to work with MODIS_IGBP land cover inputs
- Updates to biogenic VOCs and SOA for MOZART/MOSAIC
- & TBD

For questions on NCAR updates contact Mary Barth, Gabriele Pfister, Alma Hodzic, Stacy Walters, John Wong

- ***Chem session is Thursday morning***
- ***Posters are Wednesday afternoon***
- ***Developers meeting at lunch today***
- ***Publication list now online***

http://ruc.noaa.gov/wrf/WG11/References/WRF-Chem.references_Apr2012.htm

Please use this list to find papers to read and cite.
Please send us your publications too!

WRF/Chem web site - http://wrf-model.org/WG11

Thank you!